

Final Report
NASA # NAG-1-1978

Fast Bound Methods for Large Scale Simulation with Application for Engineering Optimization

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Period Covered: 12/10/1997 – 12/09/2000

Date: January 28, 2002

1. Introduction

In this work, we have focused on fast bound methods for large scale simulation with application for engineering optimization. The emphasis is on the development of techniques that provide both very fast turnaround and a certificate of fidelity; these attributes ensure that the results are indeed relevant to — and trustworthy within — the engineering context. The bound methodology which underlies this work has many different instantiations: finite element approximation; iterative solution techniques; and reduced-basis (parameter) approximation. In this grant we have, in fact, treated all three, but most of our effort has been concentrated on the first and third. We describe these below briefly — but with a pointer to an Appendix which describes, in some detail, the current “state of the art.”

2. Output Bounds for Isoparametric Finite Element Discretizations of the Heat and Incompressible Stokes Equations

A priori error estimates inform us of the asymptotic rates of convergence, but cannot answer the ever present engineering question, “can I trust the current approximation?” Such questions often revolve around concerns of mesh fidelity and feature resolution — issues of numerical uncertainty which erode confidence in the simulation. As confidence erodes, so does the utility of the simulation in the engineering design process: either the simulation is not trusted, or it is more costly than necessary. We present an implicit *a posteriori* method for computing rigorous constant-free upper and lower bounds for outputs from isoparametric finite element discretizations. The error bounds significantly reduce numerical uncertainty by providing confirmation of accuracy as well as allowing for the effective trade-off between accuracy and computational cost. The method relies on a partition of unity which decomposes the domain into independent nodal patch Neumann subproblems. We apply the method to both the heat and Stokes equations posed on two-dimensional domains with curved boundaries. See Appendix I for a description of the methodology and some application.

2. Reduced-Basis Output Bound Methods

We present a technique for the rapid and reliable prediction of linear-functional outputs of elliptic (and parabolic) partial differential equations with affine parameter dependence. The essential components are (i) (provably) rapidly convergent global reduced-basis approximations — Galerkin projection onto a space W_N spanned by solutions of the governing partial differential equation at N selected points in parameter space; (ii) *a posteriori* error estimation — relaxations of the error-residual equation that provide inexpensive yet sharp and rigorous bounds for the error in the outputs of interest; and (iii) off-line/on-line computational procedures — methods which decouple the generation and projection stages of the approximation process. The operation count for the on-line stage — in which, given a new parameter value, we calculate the output of interest and associated error bound — depends only on N (typically very small) and the parametric complexity of the problem; the method is thus ideally suited

for the repeated and rapid evaluations required in the context of parameter estimation, design, optimization, and real-time control. See Appendix II for a description of the methodology and some application.

3. Publications

Maday, Y., Patera, A.T., and Peraire, J., 1999, "A general formulation for *a posteriori* bounds for output functionals of partial differential equations; application to the eigenvalue problem," *C. R. Acad. Sci. Paris, Série I*, **328**, pp. 823–828.

Machiels, L., Maday, Y., and Patera, A.T., 2000, "A "flux-free" nodal Neumann subproblem approach to output bounds for partial differential equations", *C. R. Acad. Sci. Paris, Série I*, **330**, pp. 249–254.

Maday, Y., Patera, A.T., and Peraire, J., 1999, "A general formulation for *a posteriori* bounds for output functionals of partial differential equations; Application to the eigenvalue problem," *C. R. Acad. Sci. Paris, Serie I*, **328**, pp. 823–828.

Machiels, L., Maday, Y., Oliveira, I.B., Patera, A.T., and Rovas, D.V., 2000, "Output bounds for reduced-basis approximations of symmetric positive definite eigenvalue problems," *C. R. Acad. Sci. Paris, Serie I*, **331**(2), pp. 153–158.

Maday, Y., Machiels, L., Patera, A.T., and Rovas, D.V., 2000, "Blackbox reduced-basis output bound methods for shape optimization," In *Proceedings 12th International Domain Decomposition Conference*, pp. 429–436, Chiba, Japan.

Maday, Y. and Patera, A.T., 2000, "Numerical analysis of *a posteriori* finite element bounds for linear functional outputs," *Math. Mod. Meth. Appl. Sci.*, **10**(5), pp. 785–799.

Paraschivoiu, M. and Patera, A.T., 2000, "*A posteriori* bounds for linear functional outputs of Crouzeix-Raviart finite element discretizations of the incompressible Stokes problem," *Int. J. Numer. Meth. Fluids*, **32**(7), pp. 823–849.

Maday, Y., Patera, A.T., and Rovas, D.V., 2001, "A blackbox reduced-basis output bound method for noncoercive linear problems," *Nonlinear Partial Differential Equations and Their Applications*, Proceedings of the College De France Seminars.

Patera, A.T. and Ronquist, E.M., 2001, "A general output bound result: Application to discretization and iteration error estimation and control," *Math. Mod. Meth. Appl. Sci.*, **11**(4), pp. 685–712.

Machiels, L., Maday, Y., and Patera, A.T., 2001, "Output bounds for reduced-order approximations of elliptic partial differential equations," *Comput. Methods Appl. Mech. Engrg.*, **190**, pp. 3413–3426.

Machiels, L., Peraire, J., and Patera, A.T., 2001, “*A posteriori* finite element output bounds for the incompressible Navier-Stokes equations; Application to a natural convection problem.” *J. Comput. Phys.*, **172**, pp. 401–425.

Prud’homme, C., Rovas, D.V., Veroy, K., Machiels, L., Maday, Y., Patera, A.T. and Turinici, G., 2002, “Reliable real-time solution of parametrized partial differential equations: Reduced-basis output bound methods,” *Journal of Fluids Engineering*, accepted for publication.

Maday, Y., Patera, A.T., and Turinici, G., “*A priori* convergence theory for reduced-basis approximations of single-parameter elliptic partial differential equations,” *J. Scientific Computing*, accepted for publication.

Appendices

- Appendix I Budge, A.M., Patera, A.T., and Peraire, J. "Output bounds for isoparametric finite element discretizations of the heat conduction and incompressible Stokes flow problems," SMA-HPCES Workshop, 15–19 January 2001, Singapore.
- Appendix II Prud'homme, C., Rovas, D.V., Veroy, K., Machiels, L., Maday, Y., Patera, A.T., and Turinici, G. "Reliable real-time solution of parametrized partial differential equations: Reduced-basis output bound methods," *Journal of Fluids Engineering*, accepted for publication.